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Title: ON TIME INTEGRATION METHODS AND ERRORS FOR ASCI APPLICATIONS

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Los Alamos
NATIONAL LABORATORY

ON TIME INTEGRATION METHODS AND ERRORS FOR ASCI APPLICATIONS

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ABSTRACT

This talk is one of four to be given in the Multiphysics Solution Methods section of the workshop, Methods for Computational Physics. Some background and motivation is given for the various multiphysics time integration approaches. Various splitting methods as well as more modern coupled methods are discussed. Methods for assessing solution accuracy and time integration error are discussed. Finally, important open issues are highlighted.

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On Time Integration Methods and Errors for ASCI Applications

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Talk Outline

- Some Background
- Modified Equation Analysis of Splitting Errors
- Numerical Experiments with Radiation Diffusion
  - Some current approaches
  - Issues
- Whats Next

Multiphysics Problems:

The Computational Challange

- Systems contain multiple time scales (normal modes)

  In a simple picture of radiation hydrodynamics we have the shock speed, radiation transport, and radiation material coupling.

- Required to treat fast normal modes implicitly to step over stability contraints while using time steps on order of the dynamical time scale.

- Historically tackled using linearization and time splitting for stability and efficiency.

  Nonlinear convergence within a time step was / is viewed as unnecessary.

- However, Stability $\neq$ Accuracy.

Implicitly Balanced

vs

Linearized and Time Split (1 of 2)

- **Definition:** Time dependent reaction-diffusion problem

  $$\frac{d\mathbf{u}}{dt} = \mathcal{D}(\mathbf{u})\mathbf{u} + \mathcal{R}(\mathbf{u})\mathbf{u}$$

  $\mathbf{u}$ is the dependent variable, t is time, $\mathcal{D}(\mathbf{u})$ represents the spatial discretization of a diffusion term, and $\mathcal{R}(\mathbf{u})$ represents volumetric reaction.

  In a **implicitly balanced** method, $\mathcal{R}(\mathbf{u})\mathbf{u}$ and $\mathcal{D}(\mathbf{u})\mathbf{u}$ will be evaluated at a **consistent value** of $\mathbf{u}$ when advancing $\mathbf{u}$ in time.

- This is NOT done in a linearized time split method. (The standard in most simulation codes, ASCI and SciDAC)

Implicitly Balanced

vs

Linearized and Time Split (2 of 2)

- A standard first order linearized time split method solves two linearized sub-systems

$$\frac{\mathbf{u}^* - \mathbf{u}^n}{\Delta t} = \mathcal{D}(\mathbf{u}^n)\mathbf{u}^*$$

$$\frac{\tilde{\mathbf{u}}^{n+1} - \mathbf{u}^*}{\Delta t} = \mathcal{R}(\mathbf{u}^n)\tilde{\mathbf{u}}^{n+1},$$

or the effective time step

$$\frac{\tilde{\mathbf{u}}^{n+1} - \mathbf{u}^n}{\Delta t} = \mathcal{D}(\mathbf{u}^n)\mathbf{u}^* + \mathcal{R}(\mathbf{u}^n)\tilde{\mathbf{u}}^{n+1},$$

- One possible second order accurate "coupled" approach would be

$$\frac{\mathbf{u}^{n+1} - \mathbf{u}^n}{\Delta t} = \mathcal{D}(\mathbf{u}^{n+\frac{1}{2}})\mathbf{u}^{n+\frac{1}{2}} + \mathcal{R}(\mathbf{u}^{n+\frac{1}{2}})\mathbf{u}^{n+\frac{1}{2}},$$

- $\tilde{\mathbf{u}}^{n+1} \neq \mathbf{u}^{n+1}$, Is this important and if so when ?

- We are looking at one time step, what is the result of 10^6 time steps?

Main Points

- **Operator Splitting and / or unconverged non-linearities may lead to significant long time integration errors**
  - Solution may appear physical and conserve energy
  - No measure of error in most current ASCI time integration algorithms (residual of time step is not formed)
  - Coupling of time and space errors (or at least truncation terms)
- **Removing OS / linearization does allow for larger time steps with less error when normal modes and dynamical time scale are spread**
  - Could produce lower "wall clock time" simulations.
  - Will put increase demands on linear algebra. Larger matracies and less diagionally dominant.
  - Possible decoupling of time and space errors

Modified Equation Analysis

- **Question:**

  Does better coupling produce better answers ?

- **Current Answer:**

  Coupled methods will have a different "Modified Equation " as compared to a split method. We must improve our understanding of this for ASCI problems.

- Multiple efforts have begun to ask questions in 1-D nonequilibrium diffusion. Must extend to multi-D and multi-material.

Linear Reaction - Diffusion (1 of 6)

Modified Problem Analysis (MPA) in time

- $$\frac{\partial T}{\partial t} - D\frac{\partial^2 T}{\partial x^2} = \alpha T$$

  $$T_{x=0} = T_L, \ \ T_{x=1} = T_R$$

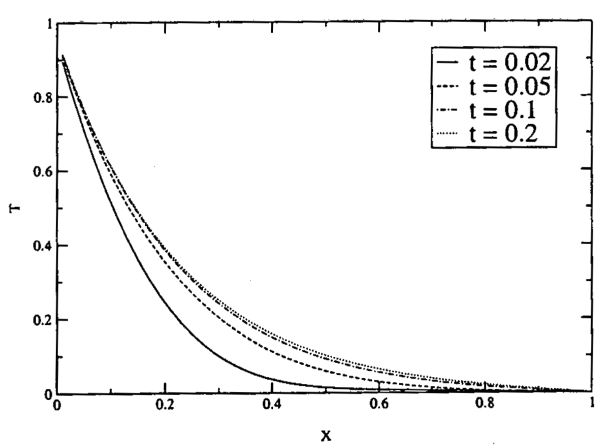
- Dynamical Time Scale

  $$\frac{1}{\tau_{dyn}} \equiv -(\frac{1}{T}\frac{dT}{dt}) = -\frac{D}{T}\frac{\partial^2 T}{\partial x^2} - \alpha \approx \frac{1}{\tau_{dif}} + \frac{1}{\tau_{reac}},$$

  $$\tau_{dif} \equiv \frac{L^2}{D} \ ; \ \tau_{reac} \equiv -\frac{1}{\alpha},$$

  and L is taken as the length of the domain.

- $T(t=0) = 0, D = 1, \alpha = -20, \Delta t = 0.01, T_L = 1, T_R = 0, \alpha\Delta t = -0.2$



Linear Reaction - Diffusion (2 of 6)

Time Integration

- First order, balanced:

$$\frac{T^{n+1} - T^n}{\Delta t} - D\frac{\partial^2 T^{n+1}}{\partial x^2} = \alpha T^{n+1}$$

$$T^{n+1}_{x=0} = T_L, \quad T^{n+1}_{x=1} = T_R$$

- First order split (R-D):

$$\frac{T^* - T^n}{\Delta t} = \alpha T^*$$

$$\frac{T^{n+1} - T^*}{\Delta t} - D\frac{\partial^2 T^{n+1}}{\partial^2 x} = 0$$

$$T^{n+1}_{x=0} = T_L, \quad T^{n+1}_{x=1} = T_R$$

- First order split (D-R):

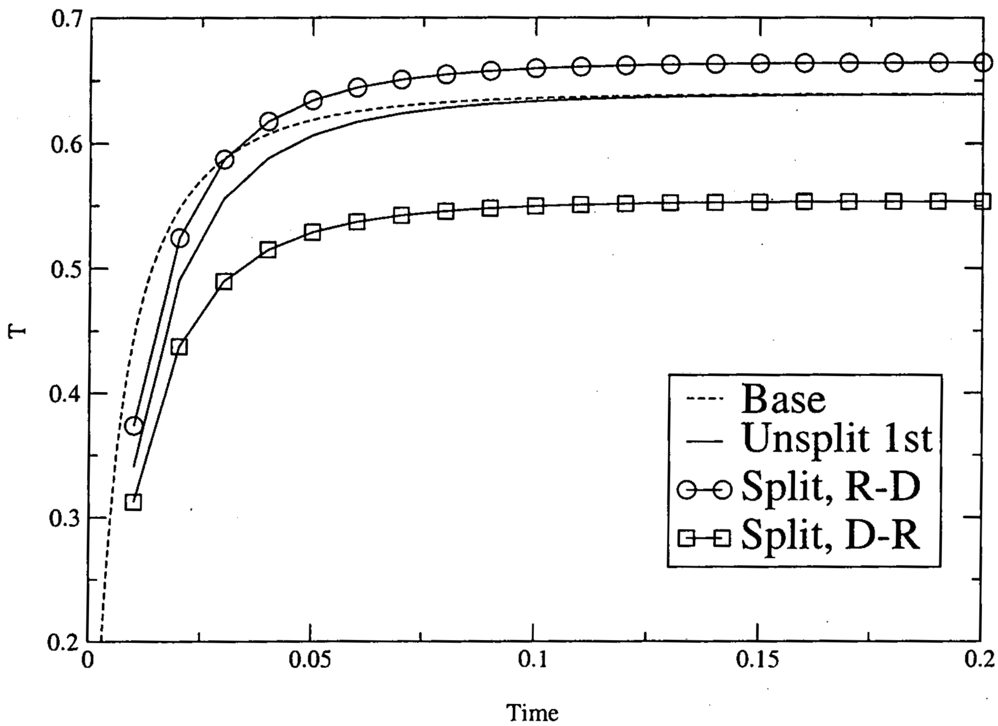
$$\frac{T^* - T^n}{\Delta t} - D\frac{\partial^2 T^*}{\partial^2 x} = 0$$

$$T^*_{x=0} = T_L, \quad T^*_{x=1} = T_R$$

$$\frac{T^{n+1} - T^*}{\Delta t} = \alpha T^{n+1}$$

Linear Reaction - Diffusion (3 of 6)

- Split solutions give the wrong steady state. D-R not equal to R-D.



- Solution DOES converge with decreasing time step.

Linear Reaction - Diffusion (4 of 6)

Modified Problem Analysis (MPA)

- MPA on First order, balanced, Yields:

$$[T_t - D\frac{\partial^2 T}{\partial x^2} - \alpha T] = \frac{\Delta t}{2}T_{tt} + O(\Delta t^2)$$

$$T_{x=0} = T_L, \quad T_{x=1} = T_R$$

- MPA on R-D splitting Yields:

$$[T_t - D\frac{\partial^2 T}{\partial x^2} - \alpha T] = \frac{\Delta t}{2}T_{tt} + \underline{\Delta t \alpha D\frac{\partial^2 T}{\partial x^2}} + O(\Delta t^2)$$

$$T_{x=0} = T_L, \quad T_{x=1} = T_R$$

- MPA on D-R splitting Yields:

$$[T_t - D\frac{\partial^2 T}{\partial x^2} - \alpha T] = \frac{\Delta t}{2}T_{tt} + \underline{\Delta t \alpha D\frac{\partial^2 T}{\partial x^2}} + O(\Delta t^2)$$

$$T_{x=0} = \underline{T_L/(1 - \alpha \Delta t)}$$

$$T_{x=1} = \underline{T_R/(1 - \alpha \Delta t)}$$

- Splitting errors scale with $\alpha \Delta t$, normal mode.

Linear Reaction - Diffusion (5 of 6)

Results

- New first-order truncation term in R-D splitting looks like diffusion.
- Use D^* in R-D splitting and equate the resulting modified equation to the modified equation from first order unsplit to get:

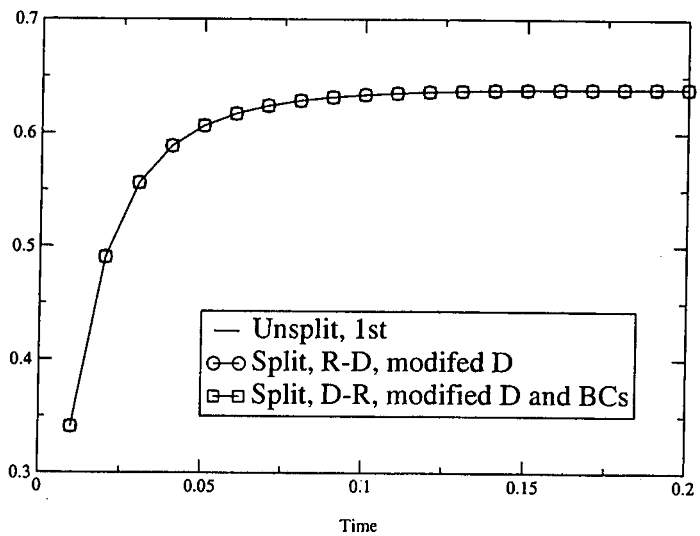
$$D^* = \frac{D}{1.0 - \Delta t \alpha}$$

- What is the result of using D^* in R-D split simulation ?
- D-R splitting has introduced an additional error in the BCs
- What is the result of using D^* and modified BCs in D-R split simulation ?

Linear Reaction - Diffusion (6 of 6)

Results

- For this simple problem, I can adjust the diffusion coefficient (and boundary conditions for D-R) to force the split method to produce the unsplit solution.



- These start to look like “Knobs”

- What if I was using the split solver to simulate an experiment ?

Numerical Experiments with Radiation Diffusion

- This 1-D model problem serves as a starting point for studying nonequilibrium thermal wave.

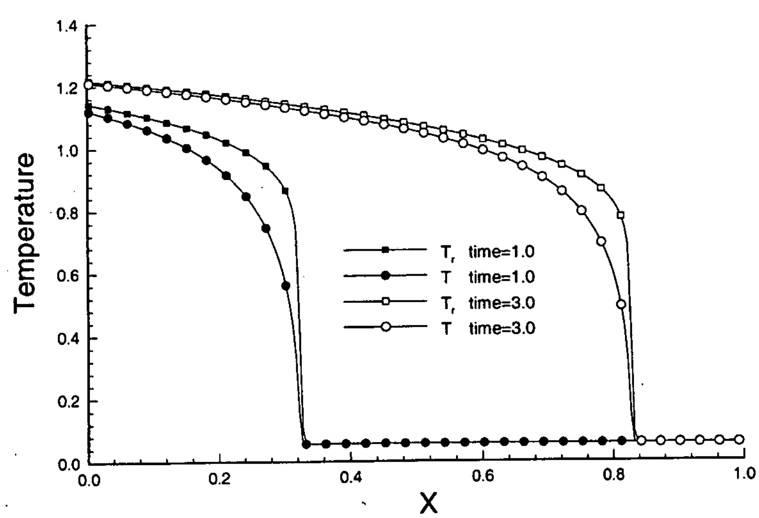
$$\frac{\partial E}{\partial t} - \frac{\partial}{\partial x}(D_r \frac{\partial E}{\partial x}) = \sigma_a(T^4 - E), \tag{1}$$

$$\frac{\partial T}{\partial t} = -\sigma_a(T^4 - E), \tag{2}$$

$$\sigma_a = T^{-3}, \quad D_r(T, E) = \frac{1}{(3\sigma_a + \frac{1}{E}|\frac{\partial E}{\partial x}|)}.$$

- Time scales: τ_{dyn}, the thermal front propagation on the grid, and $\tau_{reac} \approx \frac{1}{\sigma_a}$ near the front.

- Knoll, Rider, and Olson. *J. Quant. Spec. Rad. Tran.*, **63**, 15-29 (1999), and *J. Quant. Spec. Rad. Tran.*; **70**, 25-36 (2001)



Some Existing Approaches

- Consider a simple nonequilibrium radiation diffusion model problem. (linear BC, Fixed E)
- We will use this as a STARTING POINT to compare and contrast current approaches
- Subtle (but important) details are left out of this presentation
- An example of a simple extension will be shown

Approach 1

- Evaluate D_r and σ_a at time level t^n
- Linearize T^4 as $(T^{n+1})^4 \approx (T^n)^4 + 4(T^n)^3(T^{n+1} - T^n)$
- The coupled LINEAR problem is then

$$\frac{E^{n+1} - E^n}{\Delta t} - \frac{\partial}{\partial x}(D_r^n \frac{\partial E^{n+1}}{\partial x}) =$$

$$\sigma_a^n([(T^n)^4 + 4(T^n)^3(T^{n+1} - T^n)] - E^{n+1})$$

$$\frac{T^{n+1} - T^n}{\Delta t} = -\sigma_a^n([(T^n)^4 + 4(T^n)^3(T^{n+1} - T^n)] - E^{n+1})$$

- Evaluate for T^{n+1} and substitute into E equation

$$T^{n+1} = AE^{n+1} + B$$

$$\frac{E^{n+1} - E^n}{\Delta t} - \frac{\partial}{\partial x}(D_r^n \frac{\partial E^{n+1}}{\partial x}) = CE^{n+1} + D$$

- Solve the parabolic equation implicitly for E^{n+1}
- With E^{n+1} known, evaluate T^{n+1}.

Approach 1, cont.

- Asymptotically this linearized method is first order and does conserve energy.
- Known problems: temperature spikes at "large" Δt without iteration
- Standard time step control

  Monitor $\frac{\Delta E}{E}$
- Could iterate based on error in T^4 linearization

$$\frac{(T^{n+1})^4 - [(T^n)^4 + 4(T^n)^3(T^{n+1} - T^n)]}{(T^{n+1})^4}$$

Approach 2

- Combine discrete equations to eliminate T^4

$$\frac{E^{n+1} - E^n}{\Delta t} - \frac{\partial}{\partial x}(D_r^n \frac{\partial E^{n+1}}{\partial x}) = \frac{T^{n+1} - T^n}{\Delta t}$$

- Write down analytical solution for (linearized) temperature ODE in terms of $\phi = T^4$ with E^{n+1} as a parameter

$$\frac{dT}{dt} = \sigma(E^{n+1} - T^4)$$

goes to

$$\tau \frac{d\phi}{dt} = E^{n+1} - \phi$$

with

$$\tau = \frac{1}{\sigma T^3}$$

- Solution is

$$\phi(E^{n+1}) = \phi_o + (1 - \alpha)(E^{n+1} - \phi_o)$$

with

$$\alpha = exp(\frac{-\Delta t}{\tau})$$

Approach 2, cont.

- Approximate T^{n+1} with

$$T^{n+1} \approx T^n + \frac{\partial T}{\partial E}(E^{n+1} - E^n)$$

- Compute $\frac{\partial T}{\partial E}$ from $\phi(E^{n+1})$ to get

$$T^{n+1} = AE^{n+1} + B$$

- Substitute into E equation and solve implicitly

$$\frac{E^{n+1} - E^n}{\Delta t} - \frac{\partial}{\partial x}(D_r^n \frac{\partial E^{n+1}}{\partial x}) = CE^{n+1} + D$$

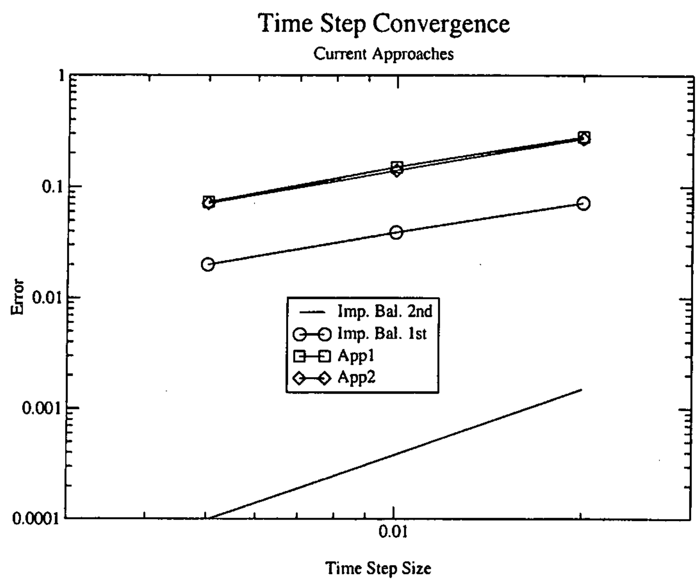
- Evaluate $T^{n+1} = AE^{n+1} + B$

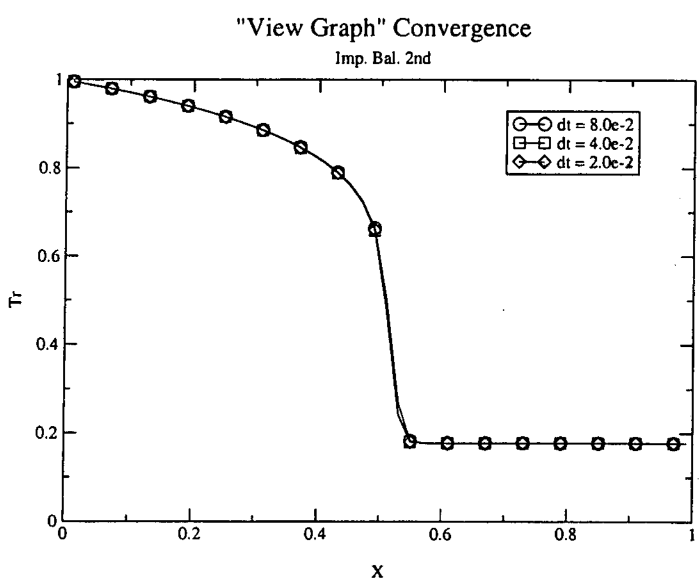
Approach 2, cont.

- Asymptotically this linearized method is first order and does conserve energy.
- Known problems: temperature spikes at "large" Δt without iteration
- Standard time step control

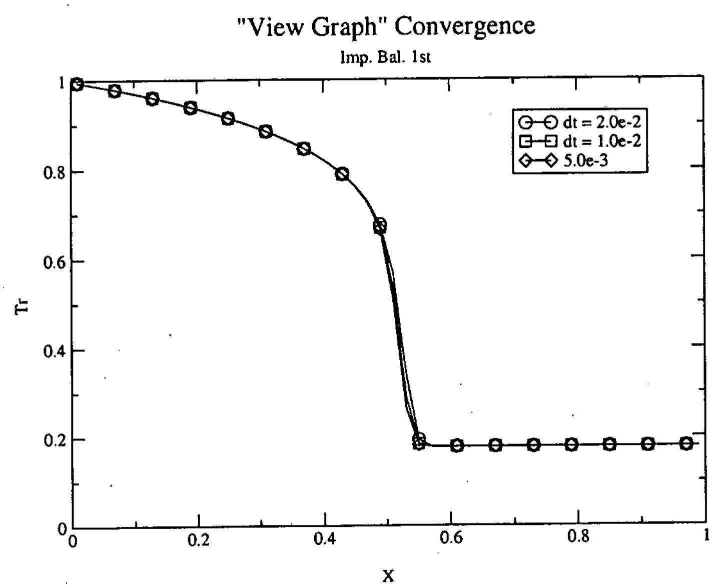
  Monitor $\frac{\Delta E}{E}$
- Could iterate based on comparing T^{n+1} with $(\phi(E^{n+1}))^{0.25}$

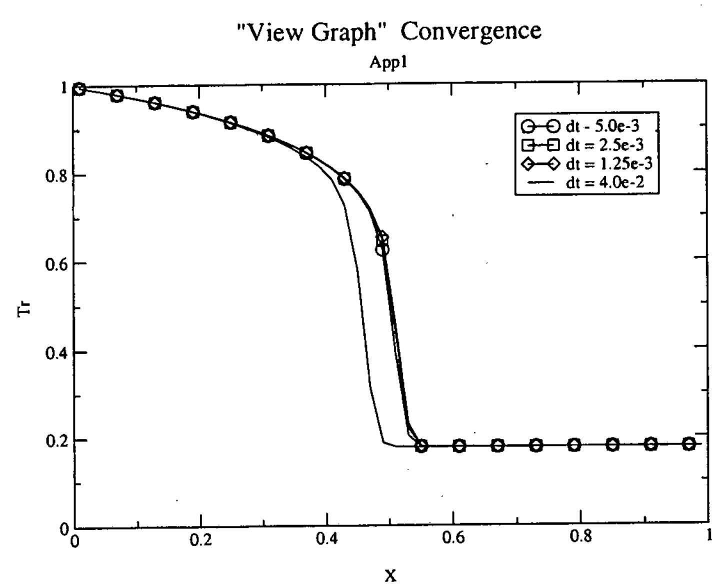
Some Results





Some Results, cont.





A Possible Simple Extention

Explict (or linear implicit) half step:

$$\frac{E^* - E^n}{\Delta t} - 0.5\frac{\partial}{\partial x}(D_r^n \frac{\partial E^n}{\partial x}) = 0$$

Coupled Nonlinear 2 x 2:

$$\frac{T^{n+1} - T^n}{\Delta t} = -0.5[(\sigma_a^{n+1}((T^{n+1})^4 - E^{**})) + (\sigma_a^n((T^n)^4 - E^*))]$$

$$\frac{E^{**} - E^*}{\Delta t} = -0.5[(\sigma_a^{n+1}((T^{n+1})^4 - E^{**})) + (\sigma_a^n((T^n)^4 - E^*))]$$

Implicit (linear) half step:

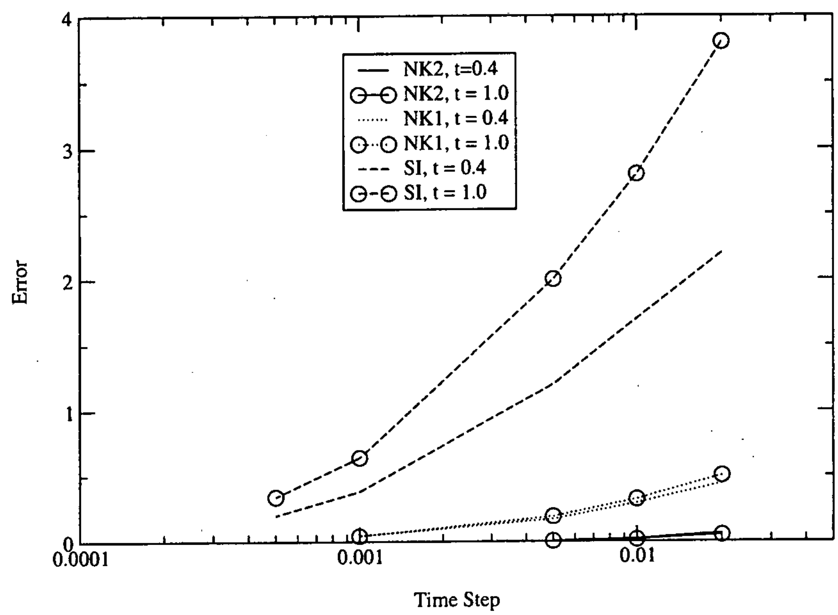
$$\frac{E^{n+1} - E^{**}}{\Delta t} - 0.5\frac{\partial}{\partial x}(D_r^{n+1} \frac{\partial E^{n+1}}{\partial x}) = 0$$

- Considered by Shadid et. al.
- Nonlinear solves are local, but iterate on σ_a and T^4.
- Similar to Strang 2nd order splitting

Nonequilibrium Radiation Diffusion (1 of 2)

Error Accumulation in time

- How does the linearization error accumulate in time ?

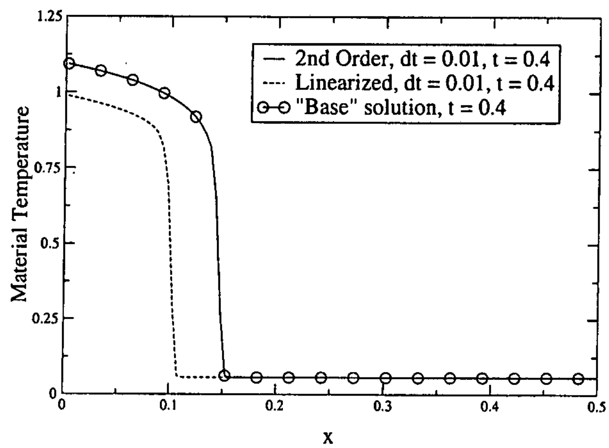


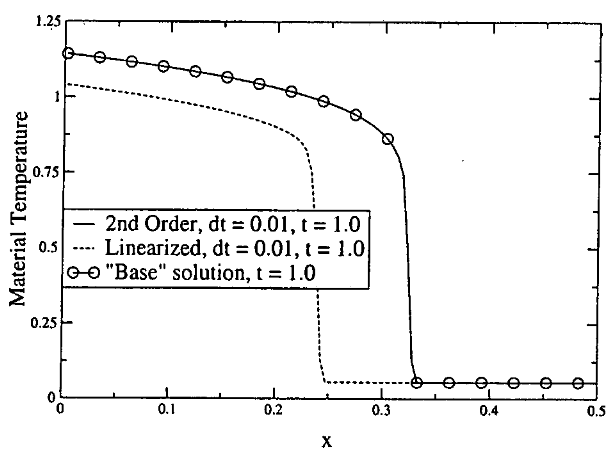
- We observe a significant accumulation of error from $t = 0.4$ to $t = 1.0$. $t = 1.0$ is only 100 time steps !

Nonequilibrium Radiation Diffusion (2 of 2)

Predictive Simulation

- How does error accumulation in time effect PREDICTIVE capability ?





- There is a relationship between error accumlation per time step, problem nonlinearity, and number of time steps.

Issues To Consider

1. Split vs Coupled

2. Unconverged nonlinearities

3. 1st vs 2nd order in time

4. Interaction of time and space errors

5. Long time integration error growth

We know very little about point 5 and it is crucial to contructing effective time step control methods. Require an increased research effort.

Whats Next ?

- Characterize current approaches and consider simple improvements / extensions

- Move numerical experiments into 2-D, multi-material, and consider wider range in τ_{dyn}. Understand possible interations between time and space errors with splitting and linearization.

- Move MEA from 1-D linear scaler to 1-D nonlinear systems. Study long time integration errors. Consider issues of discontinuities and table look ups.

- Basic algorithms work